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Title: Polycrystal Models of Irradiation and Thermal Creep of Cladding

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Section: Modeling and Simulation
Topic: Fuels Modeling
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"Polycrystal models of irradiation and thermal creep of cladding"

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ABSTRACT
Irradiation-generated vacancies and interstitials migrate to dislocations and dislocation loops, inducing dislocation climb. Such process produces irradiation and thermal creep, and is responsible for the dimensional changes observed in cladding. As a consequence, modeling creep is central to predicting deformation of cladding during reactor operation.

Cladding is an aggregate of crystallographic grains (i.e. austenitic steel or zirconium alloy). These grains exhibit an orientation distribution (texture) induced by the manufacturing process, and the dislocations inside the grains exhibit well defined orientations with respect to the grain axes. As a consequence, creep is a directional process, dependent on the grains' orientations and on the grain-to-grain interactions. Crystallographic models have the double advantage that they are based on the actual mechanism of dislocation climb and glide, and that they account for the directionality of creep (anisotropy).

We use an Effective Medium Polycrystal Model to simulate irradiation and thermal creep of cladding. In this paper we will give a brief overview of the model, will show predictions of creep, and will discuss how this constitutive description can be incorporated in Finite Element codes used for large-scale fuel element simulations.

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Section: Modeling and Simulation
Topic: Fuels Modeling
Date: Tuesday May 17, 10:15 am.

Polycrystal models of irradiation and thermal creep of cladding

Carlos N. Tome
MST-8 - LANL

Work performed within Advanced Fuel Cycle Program (AFC) and Consortium for Advanced Simulation of LWR's Program (CASL)

LANL Nuclear Engineering Review

Modeling mechanical response of Zrly cladding under irradiation

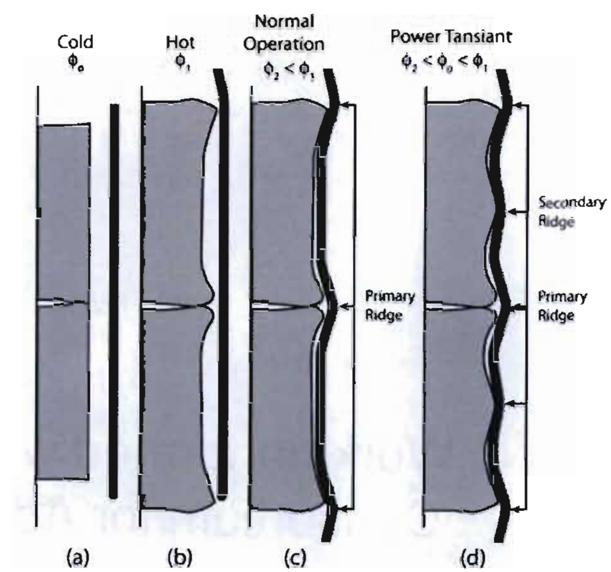
1- Irradiation Creep (stress driven)
→ ongoing modeling effort

2- Irradiation Growth (no stress required)
→ ongoing modeling effort

3- Thermal Creep (stress driven)
→ ongoing modeling effort

4- Fracture and Corrosion
(degradation of mech ppties)
→ presently not being done

Pellet-Clad Interaction:



Scales and techniques involved in modeling

Molecular dynamics

Kinetic Monte Carlo

Interstitial & vacancy diffusion and interaction with dislocations

Dislocation Dynamics

Crystal Model

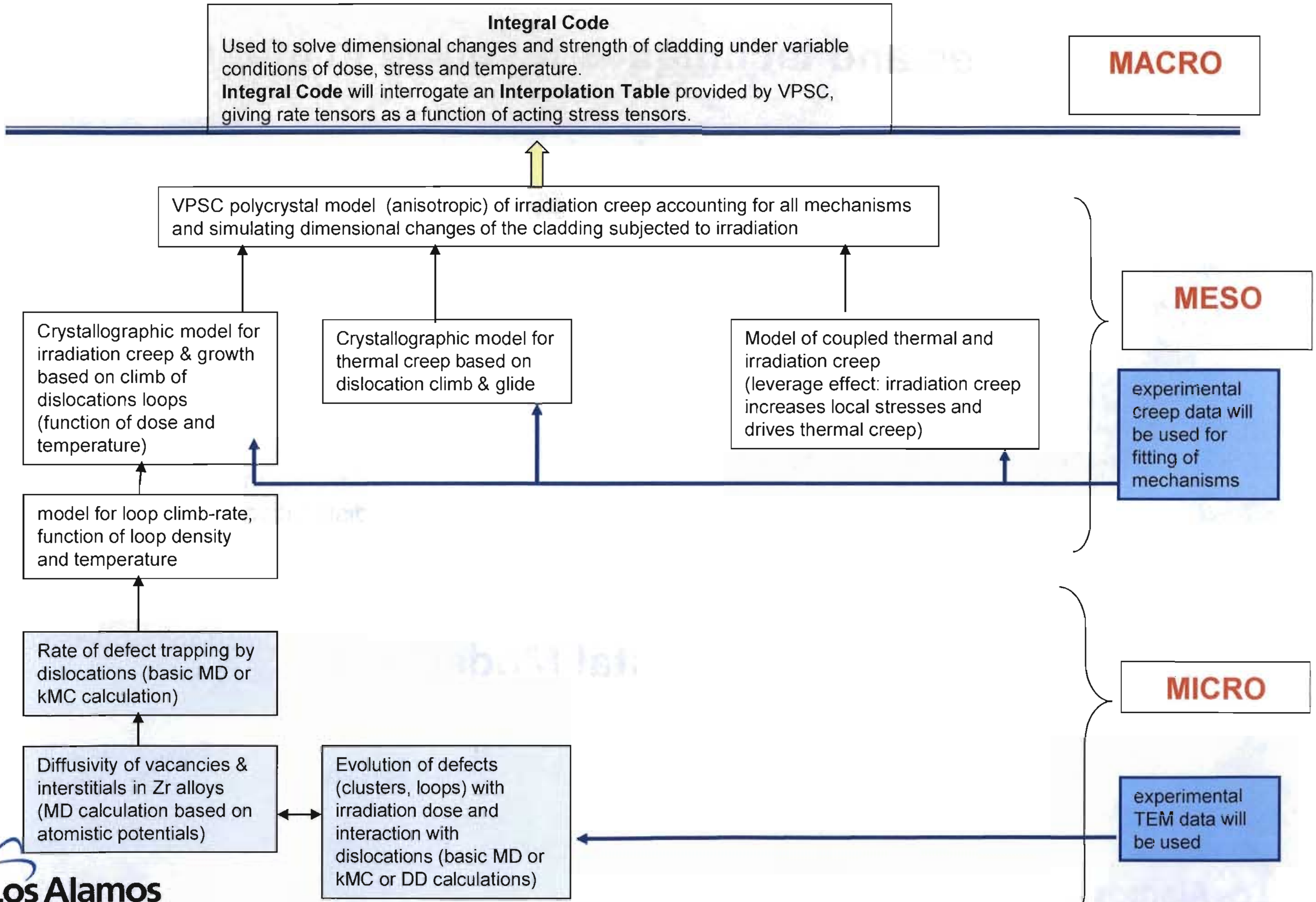
dislocation interactions, dislocation climb, creep

Polycrystal Model

Creep and hardening response

Integral FEM Code

Response of full cladding element



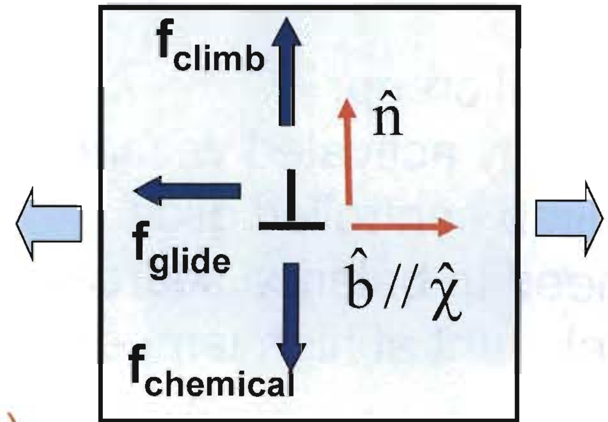
Integral Code
Used to solve dimensional changes and strength of cladding under variable conditions of dose, stress and temperature.
Integral Code will interrogate an **Interpolation Table** provided by VPSC, giving rate tensors as a function of acting stress tensors.
MACRO
VPSC polycrystal model (anisotropic) of irradiation creep accounting for all mechanisms and simulating dimensional changes of the cladding subjected to irradiation
MESO
Crystallographic model for irradiation creep & growth based on climb of dislocations loops (function of dose and temperature)
Crystallographic model for thermal creep based on dislocation climb & glide
Model of coupled thermal and irradiation creep (leverage effect: irradiation creep increases local stresses and drives thermal creep)
experimental creep data will be used for fitting of mechanisms
model for loop climb-rate, function of loop density and temperature
Rate of defect trapping by dislocations (basic MD or kMC calculation)
MICRO
Diffusivity of vacancies & interstitials in Zr alloys (MD calculation based on atomistic potentials)
Evolution of defects (clusters, loops) with irradiation dose and interaction with dislocations (basic MD or kMC or DD calculations)
experimental TEM data will be used

Forces acting on a dislocation: climb and glide

* Peach-Koehler (stress related)

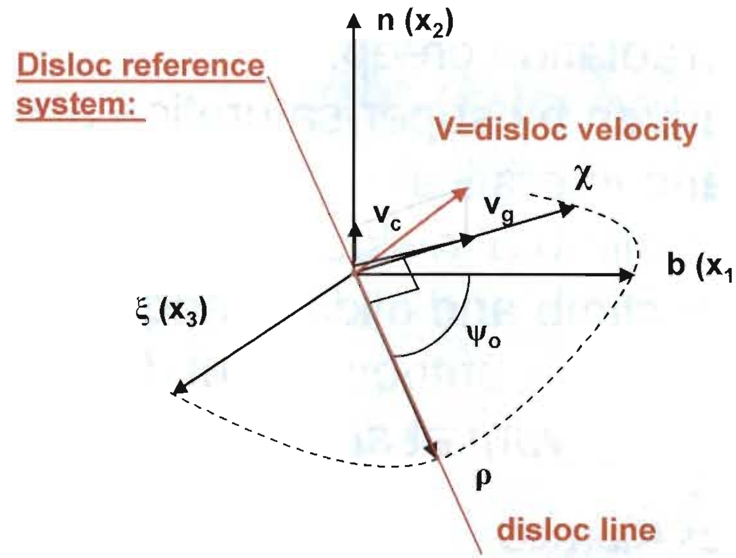
$$f_{glide} = |\mathbf{b}|\,\sigma' : \left(\hat{\mathbf{b}} \otimes \hat{\mathbf{n}}\right)$$

$$f_{climb} = -|\mathbf{b}|\,\sigma' : \left(\hat{\mathbf{b}} \otimes \hat{\boldsymbol{\chi}}\right)$$



* Chemical force (non-equilibrium vacancies)

$$f_{climb\_chem} = \frac{k_B T}{\alpha |\mathbf{b}|^2} \log \frac{C_v}{C_v^0\big|_{P,T}} \left(\hat{\mathbf{b}} \otimes \hat{\boldsymbol{\chi}}\right)$$

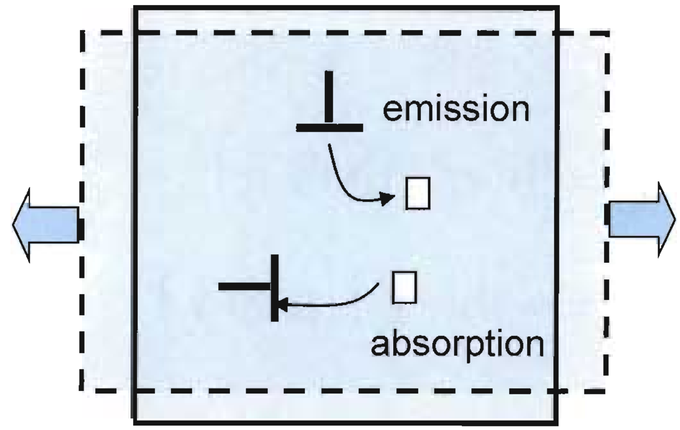


* C. Hartley, Phil Mag 83 (2003) 3783

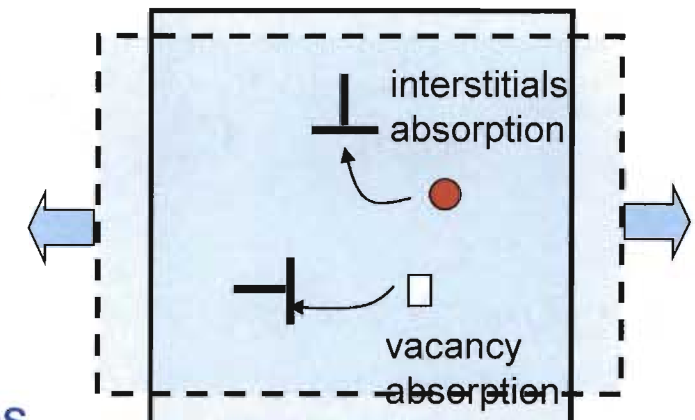
* R. Lebensohn et al, Phil Mag 90 (2010) 567

Mechanisms of thermal and irradiation creep

Thermal creep:
thermally activated vacancy diffusion
→ climb controlled glide
→ need to balance sources and sinks
→ relevant at high temperature

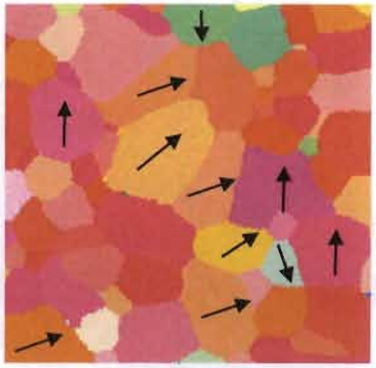


Irradiation creep:
driven by super-saturation of vacancies and interstitials
→ climb of dislocation loops
→ climb and glide of edge components of dislocations
→ relevant at all irradiation temperatures

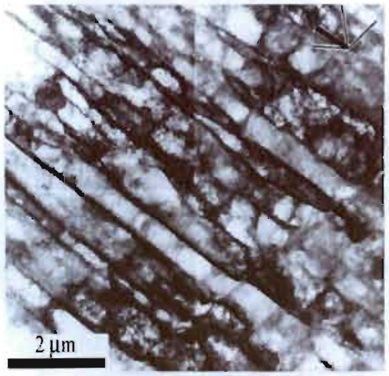


Polycrystal creep model

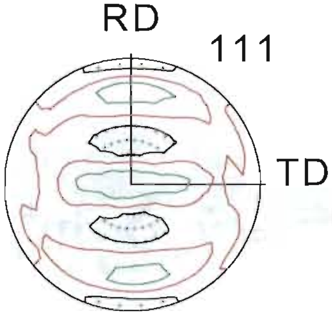
The aggregate is represented by a collection of crystal orientations with associated volume fractions chosen to reproduce the texture.



Aggregate properties are given by averages performed over the grains.



Anisotropy follows from texture (macro scale) …

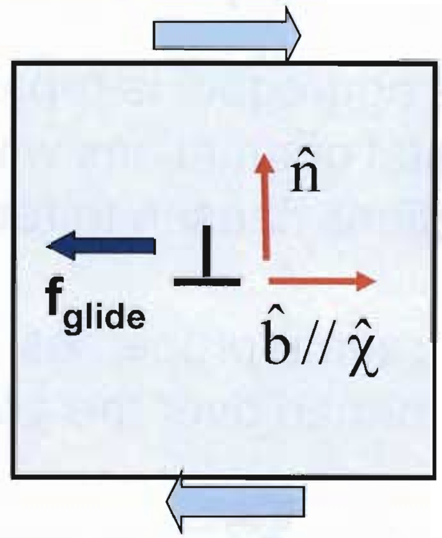


Cr steel HT9
(3000 orients)

…but also from directional microstructure features (meso scale).

Polycrystal models provide a link between macroscopic response and microstructure

Modeling thermal creep of the grain



The glide force is a resolved shear coming from the applied stress.
When the resolved shear is close to a threshold shear glide occurs

Glide tensor: $m_{ij}^{s} = n_{i}^{s} \, b_{j}^{s}$

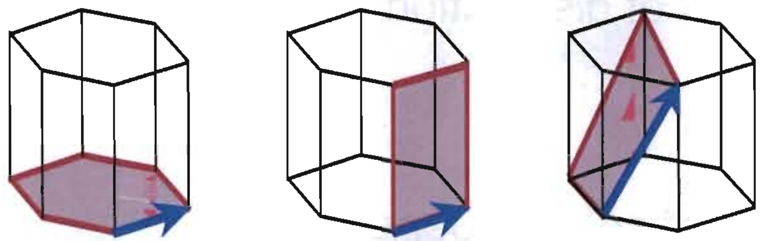
$$\dot{\varepsilon}_{ij}^{glide} = \dot{\gamma}_o \sum_s m_{ij}^{s} \left(\frac{m_{kl}^{s} \, \sigma'_{kl}}{\tau_o^{glide}} \right)^{n_g} \rho^{s}$$

Inverse of rate sensitivity → typically n_g ~3 for thermal creep

Dislocation densities already present → follow from evolution model or from experimental measurements

Threshold stress
→ function of temperature, dose, density of defects
→ follow from dislocation dynamics simulations or from fits to experimental yield stresses

Modeling thermal creep of the grain



$(0001)\langle 11\bar{2}0\rangle$ Basal slip

$(10\bar{1}0)\langle 11\bar{2}0\rangle$ Prismatic slip

$(11\bar{2}2)\langle 11\bar{2}3\rangle$ Pyramidal slip

$$\dot{\varepsilon}_{ij}^{glide} = \dot{\gamma}_o \sum_s m_{ij}^s \left(\frac{m_{kl}^s \, \sigma'_{kl}}{\tau_o^{glide}} \right)^{n_g} \rho^s$$

$$m_{ij}^s = n_i^s \, b_j^s$$

At the single crystal level, thermal creep rate is controlled by the values of dislocation densities on the different slip systems, and by the values of the threshold stresses

At the polycrystal level, thermal creep rate is further controlled by the texture of the extruded pressure tubes or cladding tubes. Extrusion is what induces the dislocation densities, different depending on the orientation of each grain.

Irradiation creep due to dislocation climb

Creep rate associated with crystallographic groups of dislocations

$$\dot{\varepsilon}_{ij}^{\,climb} = \sum_k \rho^{(k)} (\hat{l}^{(k)} \times \hat{v}^{(k)})\, b_j^{(k)} \left| v^{(k)} \right|$$

Specific case of creep rate associated with climb of sessile loops

$$\dot{\varepsilon}_{ij}^{\,climb} = \sum_k \rho^{(k)} b_i^{(k)} b_j^{(k)} \left(\Phi^{(int)} - \Phi^{(vac)} \right) \qquad = K_{ijkl}(\rho)\sigma_{kl} + \Gamma_{ij}(\rho)$$

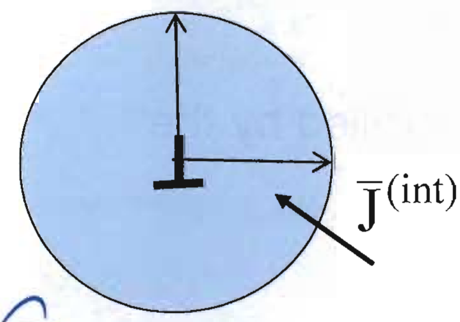
Dislocation density on different planes

Burgers vector of dislocations

Flow rate of interstitials and vacancies to dislocations

Growth rate

Creep compliance



Flow rate is given by the integral of the defect flux J around a dislocation circuit .

$$\Phi^{(int)} = \oint \bar{J}_{(\bar{x})}^{(int)} d\bar{l}$$

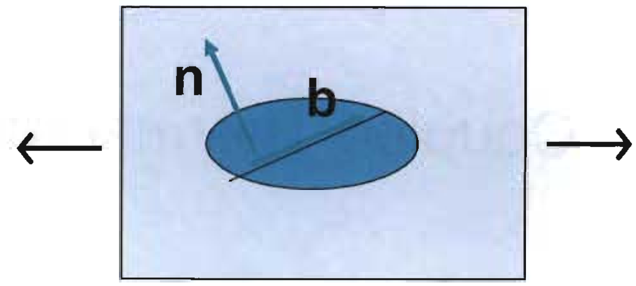
Solve using discrete approach (atomistic+Monte Carlo) or using continuum approach with anisotropic diffusivity given by atomistic

Visco-Plastic Self-Consistent (VPSC) Polycrystal Creep Model

Each grain is a visco-plastic anisotropic ellipsoidal inclusion embedded in a visco-plastic anisotropic Homogeneous Effective Medium.

Solve stress equilibrium equation for inclusion in the homogeneous medium.
→ Eshelby problem !

$$\sigma_{ij,j} = 0$$



Constitutive creep law for the grain

$$\dot{\varepsilon}_{ij}^{grain} = \dot{\varepsilon}_{ij}^{glide} + \dot{\varepsilon}_{ij}^{climb} = \dot{\gamma}_0^{gl} \sum_s m_{ij}^s \left(\frac{m_{kl}^s \sigma'_{kl}}{\tau_o^{glide}} \right)^{n_{gl}} + K_{ijkl}(\rho)\sigma_{kl} + \Gamma_{ij}(\rho)$$

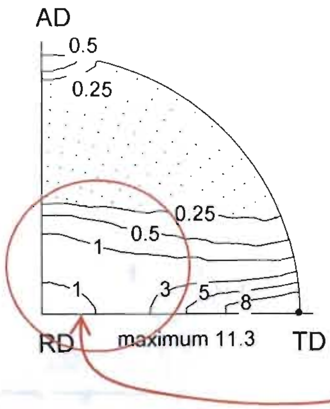
Model gives the constitutive creep law for the polycrystal : $\bar{\dot{\varepsilon}} = \overline{M} : \overline{\sigma} + \bar{\dot{\varepsilon}}_0$

and the stress and creep rate in each grain: $\dot{\varepsilon}_{ij}^{grain}$ and σ_{ij}^{grain}

Applications of Crystallographic Model

- Accelerated Irradiation Creep and Growth of Zr-Nb tubes
- Coupled Thermal Creep and Irradiation Creep of Zrly
- Creep under superimposed pressure and shear forces in SS cladding
- Yield response of irradiated SS cladding

VPSC model : Accelerated Irradiation Creep & Growth of Zr-Nb pressure tubes

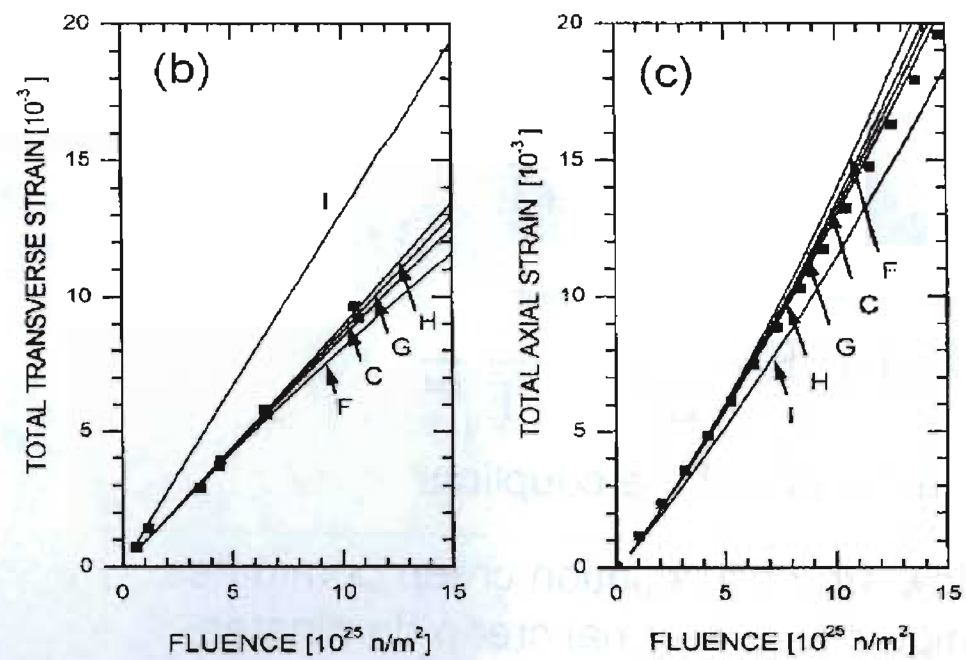


$$\rho_c(\Phi) = \left.\frac{d\rho_c}{d\Phi}\right|_0 \Delta\Phi = 1.52\ 10^{-27}\,\Delta\Phi$$

$$\rho_a(\Phi) = \left.\frac{d\rho_a}{d\Phi}\right|_0 \Delta\Phi$$

$$\rho_{c'}(\Phi) = \left.\frac{d\rho_{c'}}{d\Phi}\right|_0 \cos^2\theta\,\Delta\Phi = 0.13\,10^{-27}\cos^2\theta\,\Delta\Phi$$

Only assuming evolution of c' loops predicts the right dimensional changes… even if only a low fraction of grains contribute to this effect



C.N. Tome, N. Christodoulou, Phil. Mag. 80 (2000) 1407

Coupling thermal creep & irradiation creep

Creep terms at the single crystal level

$$\dot{\varepsilon}_{ij}^{\text{thermal}} = \dot{\gamma}_o \sum_s m_{ij}^s \left(\frac{m_{kl}^s \sigma'_{kl}}{\tau_o^{\text{thermal}}} \right)^{n_g} \rho^s \qquad \dot{\varepsilon}_{ij}^{\text{irrad}} = K_{ijkl}(\rho)\sigma_{kl} + \Gamma_{ij}(\rho)$$

Each component alone gives a polycrystal creep rate: $\dot{E}_{ij}^{\text{thermal}}$ and $\dot{E}_{ij}^{\text{irrad}}$

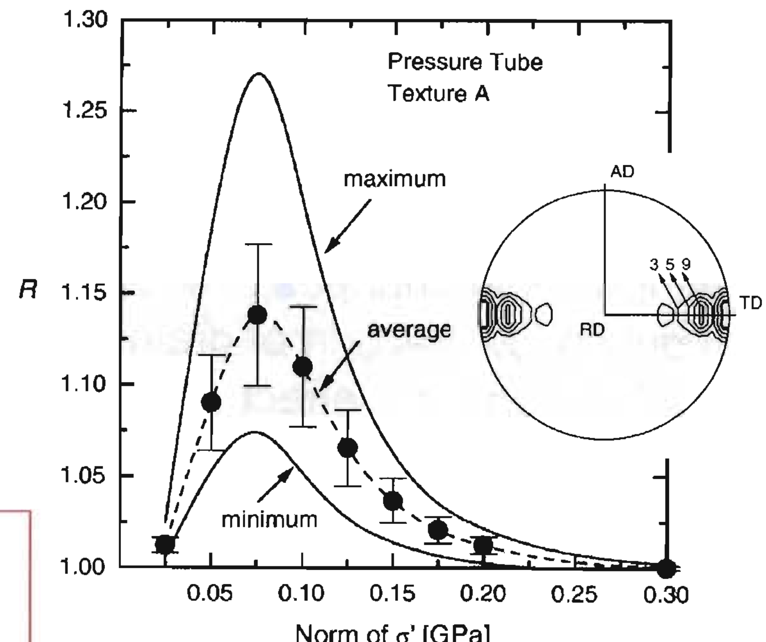
When both are acting simultaneously, they couple and give a polycrystal creep rate:

$$\dot{E}_{ij}^{\text{total}} \geq \dot{E}_{ij}^{\text{thermal}} + \dot{E}_{ij}^{\text{irrad}}$$

The ratio $R = \dfrac{\dot{E}_{ij}^{\text{total}}}{\dot{E}_{ij}^{\text{thermal}} + \dot{E}_{ij}^{\text{irrad}}}$

is a measure of the coupling.

At low stress irradiation creep dominates,
at high stress thermal creep dominates,
at intermediate stress coupling is non-negligible



Turner, Tome, Christodoulou, Woo, Philos Mag **79** (1999)

Interpolation Table approach

* The polycrystal model provides a creep rate tensor for an arbitrary applied stress tensor: $\bar{\dot{\varepsilon}} = \overline{M} : \bar{\sigma} + \bar{\dot{\varepsilon}}_0$

* Derive a database by probing the polycrystal with multiple stress states and listing the associated creep rates in a look-up Table

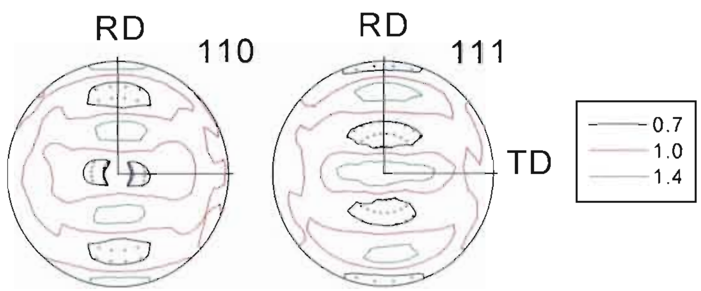
* When an arbitrary stress tensor is acting on the material, interpolate between tabulated states to infer the creep rate.

ADVANTAGE: **Retain the complexity of the Polycrystal Model and reduce the access time to the material subroutine by 2 to 3 orders of magnitude.**

DISADVANTAGE: Valid for a 'frozen' microstructure (i.e. defect densities). Devise Interpolation Approach between microstructures?

Climb and Glide Model for SS HT9

TEXTURE of Cr steel



pole figures of Cr steel HT9
RD is the axial direction (AD=X1)
TD is the circumferential direction (HD=X2)
ND is the radial direction (RD=X3) `

Glide assumed on <110> {111} dislocations (edge, screw, mix)
Climb assumed on <110> {111} dislocations (only edge component)

$$\dot{\varepsilon}_{ij}^{grain} = \dot{\varepsilon}_{ij}^{glide} + \dot{\varepsilon}_{ij}^{climb} = \dot{\gamma}_0^{gl} \sum_s m_{ij}^s \left(\frac{m_{kl}^s \, \sigma'_{kl}}{\tau_o^{glide}} \right)^{n_{gl}} + \dot{\gamma}_0^{cl} \sum_s c_{ij}^s \left(\frac{c_{kl}^s \, \sigma'_{kl}}{\tau_o^{climb}} \right)^{n_{cl}}$$

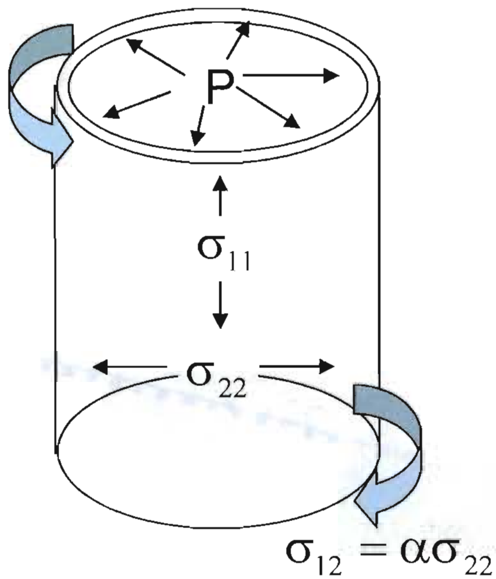
$$\dot{\gamma}_0^{gl} = \dot{\gamma}_0^{cl} = 10^{-4} s^{-1}$$

$$\tau_o^{glide} = 100\text{MPa} \quad ; \quad n_{gl} = 4$$

$$\tau_o^{climb} = 10\text{MPa} \quad ; \quad n_{cl} = 1$$

Generate the Interpolation Table for this texture and these parameters

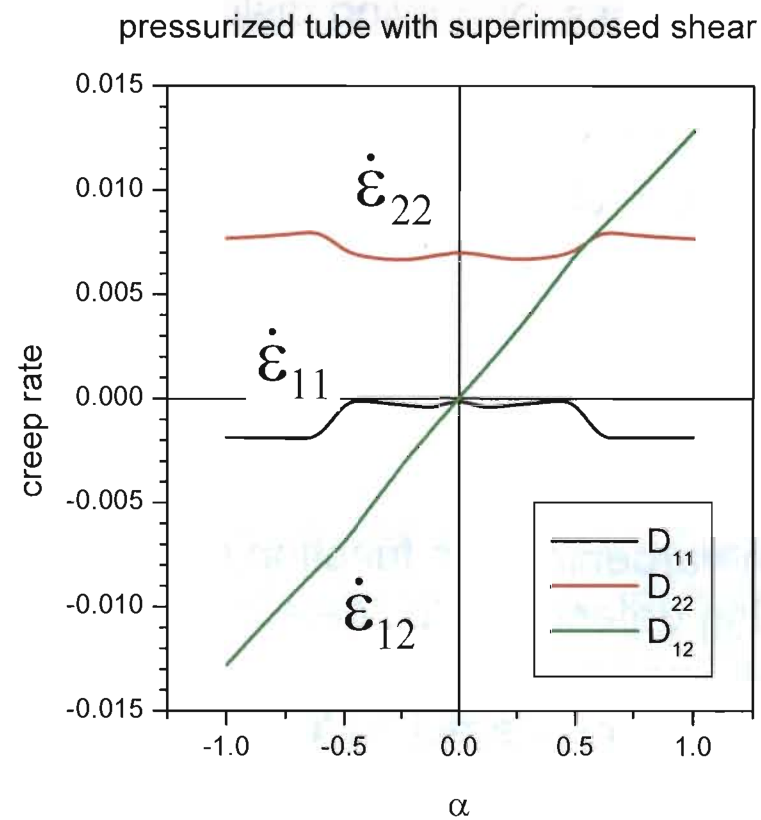
Interpolation Table Application to HT9 cladding: Creep of pressurized tube with superimposed shear



$$\sigma_{11} = P\,{}^{r}\!/_{2t} = 50\text{MPa}$$

$$\sigma_{22} = P\,{}^{r}\!/_{t} = 100\text{MPa}$$

$$\sigma_{12} = \alpha\sigma_{22} \quad (-1 < \alpha < 1)$$



The superimposed shear enhances the creep rate in the hoop and in the axial directions

Tensile deformation of irradiated SS 316L

The critical stress for moving dislocation contains a forest and an irradiation hardening term

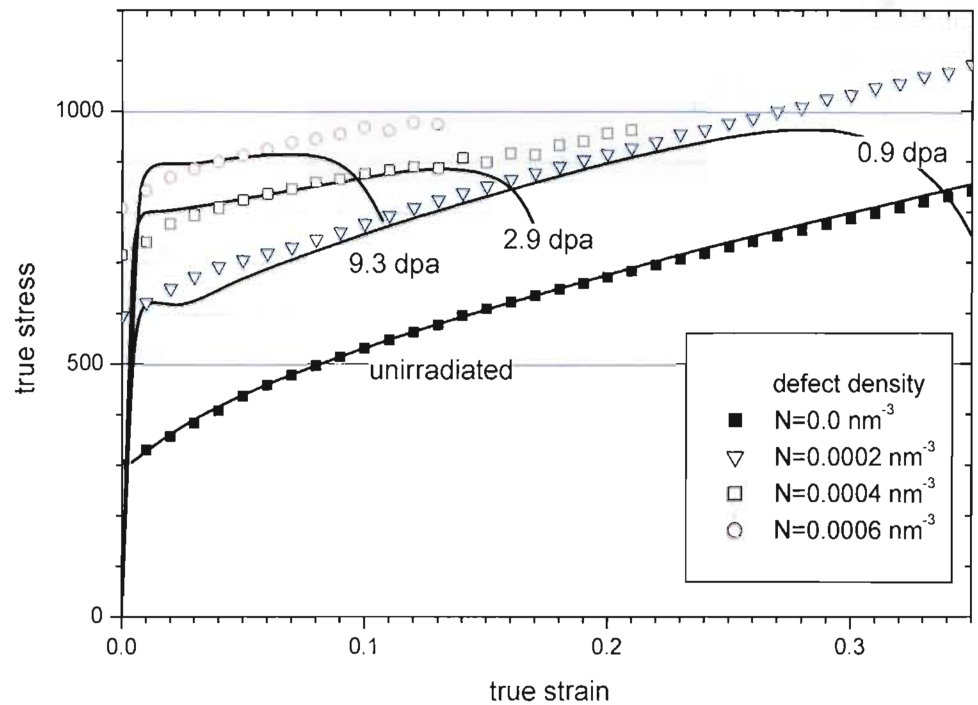
Forest hardening is a function of the shear 'Γ' accumulated in each grain

$$\tau^{\text{forest}} = \tau_0 + (\tau_1 + \theta_1 \Gamma)\left\{1 - \exp\left(-\frac{\Gamma\theta_0}{\tau_1}\right)\right\}$$

Irradiation hardening is a function of the evolving defect size 'd', defect density 'N' , and strength of dislocation-defect interaction 'α'

$$\tau^{\text{irrad}} = \alpha\mu b\sqrt{N.d}$$

Annealed 316L irradiated in spallation environment
Preliminary modeling results



The polycrystal simulation of tension reproduces the observed response of 316L irradiated to different doses